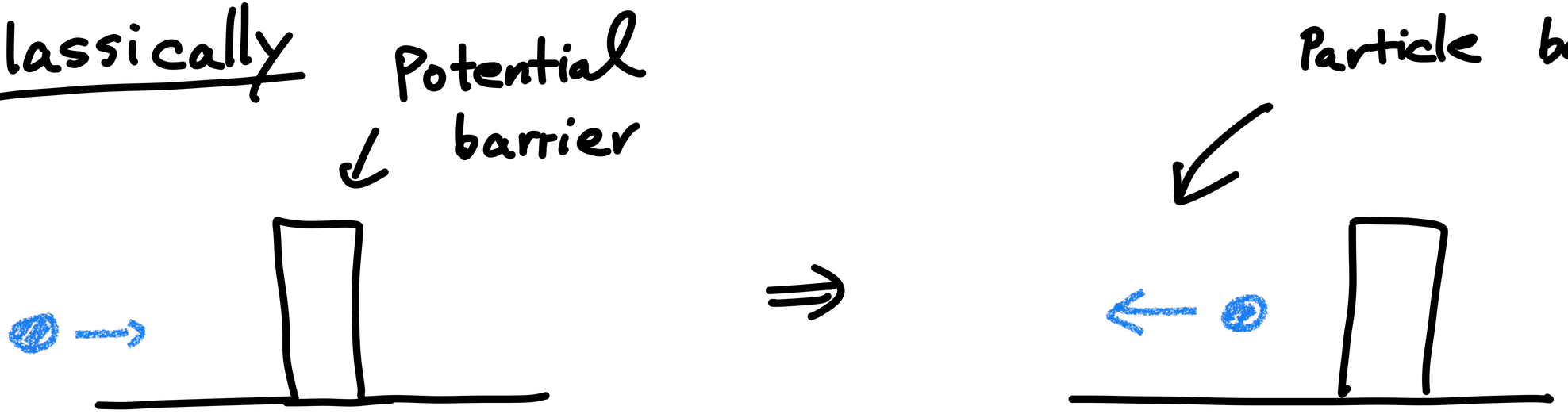
Some idea on quantum tunneling from Lefschetz thimbles

Yuya Tanizaki (YITP, Kyoto)

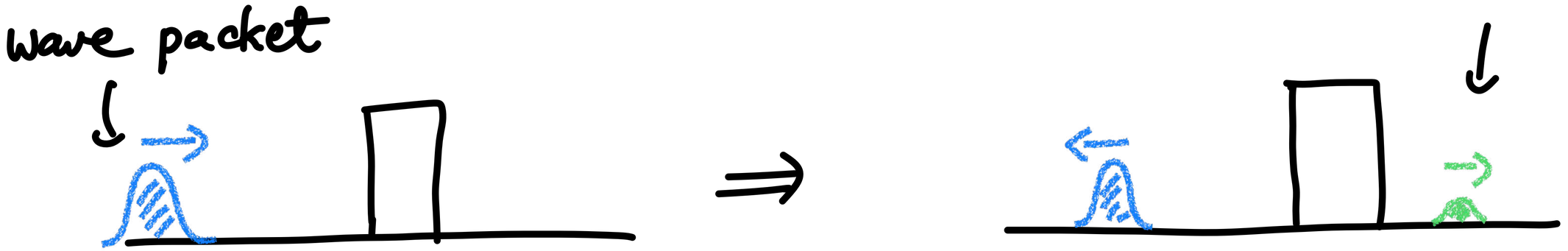
Based on 1406.2386 with Takayuki Koike

Quantum Tunneling

Classically



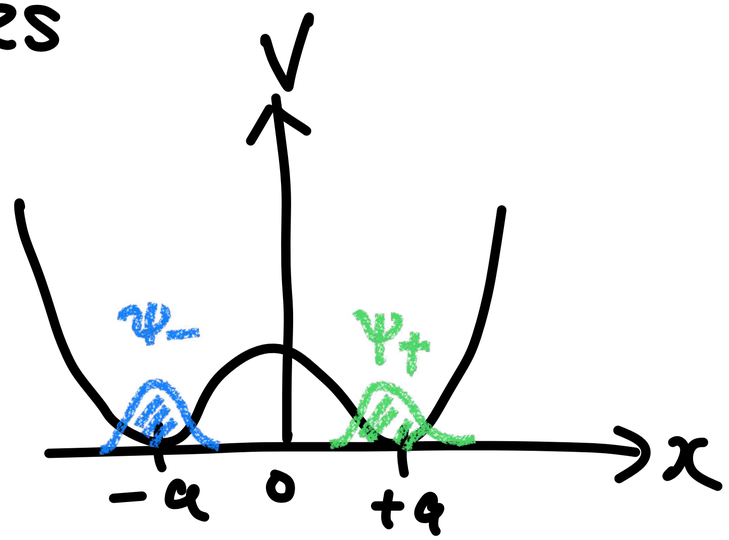
Quantum Mechanically



Tunneling and Ground States

Let's consider G.S. for the double well

$$\hat{H} = -\frac{1}{2}\partial_x^2 + \underbrace{\frac{g}{4}(x^2-a^2)^2}_{V(x)}.$$



Classical vacua of $V(x)$: $x = \pm a$ $(V(\pm a) = 0)$.

So, are there <u>two</u> ground states, ψ_+ and ψ_-?

No $\psi_{G.S.} \simeq \frac{1}{\sqrt{2}}(\psi_+ + \psi_-)$ is the true one!

Why is this so?

Standard trick

- Consider the (imaginary-time) operator: $e^{-\beta \hat{H}}$.

  G.S. of $\hat{H}$ $\Leftrightarrow$ Maximal eigenstate of $e^{-\beta \hat{H}}$.

- Assume $|\Psi_\pm\rangle$ are good approximation of low-E spectra.

  Then, compute 2x2 transition matrix:

$$\begin{pmatrix} \langle\Psi_+|e^{-\beta\hat{H}}|\Psi_+\rangle & \langle\Psi_+|e^{-\beta\hat{H}}|\Psi_-\rangle \\ \langle\Psi_-|e^{-\beta\hat{H}}|\Psi_+\rangle & \langle\Psi_-|e^{-\beta\hat{H}}|\Psi_-\rangle \end{pmatrix} \simeq \begin{pmatrix} 1 & c \to 0 \\ c & 1 \end{pmatrix}$$

- Now, let's diagonalize the 2×2 matrix $\begin{pmatrix} 1 & c \\ c & 1 \end{pmatrix}$:

$$|\psi_{G.S}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \leftarrow |\psi_+\rangle, \quad \text{eigenvalue} = 1+c \simeq e^{-\beta E_{G.S.}}$$

$$|\psi_{1st}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \leftarrow |\psi_-\rangle, \quad \text{eigenvalue} = 1-c \simeq e^{-\beta E_{1st.}}$$

- $\Delta E = E_{1st} - E_{G.S.} \ll 1$.

$$\Rightarrow \Delta E = \frac{1}{2\beta} C = \frac{1}{2\beta} \langle \psi_+ | e^{-\beta \hat{H}} | \psi_- \rangle \sim \frac{1}{2} e^{-\frac{S_{inst}}{\hbar}}.$$

instanton amplitude $\sim \beta e^{-S_{inst}/\hbar}$

Tunneling and imaginary time (Instanton)

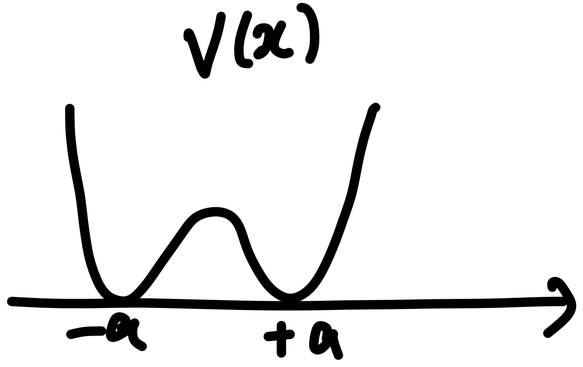
Real-time propagation

$$\langle \psi_+ | e^{-i\hat{H}T} | \psi_- \rangle = \int \mathcal{D}x \; \exp\left(i \int_0^T dt \left\{ \frac{1}{2} \left(\frac{\partial x}{\partial t} \right)^2 - V(x) \right\} \right)$$

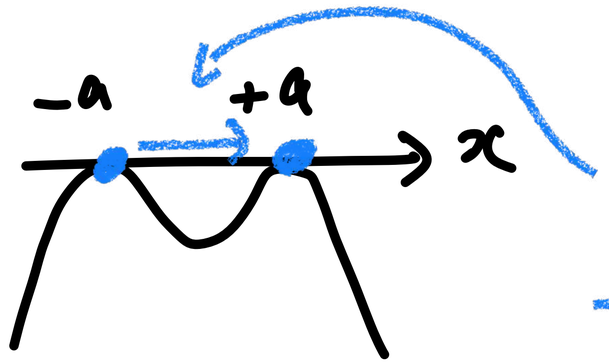
Imaginary time

$$\Downarrow \quad t \to -i\tau \,, \quad T \to -i\beta$$

$$\langle \psi_+ | e^{-\hat{H}\beta} | \psi_- \rangle = \int \mathcal{D}x \exp\left(- \int_0^\beta d\tau \left\{ \frac{1}{2} \left(\frac{\partial x}{\partial \tau} \right)^2 + V(x) \right\} \right)$$



$\Longrightarrow$



Potential is inverted.

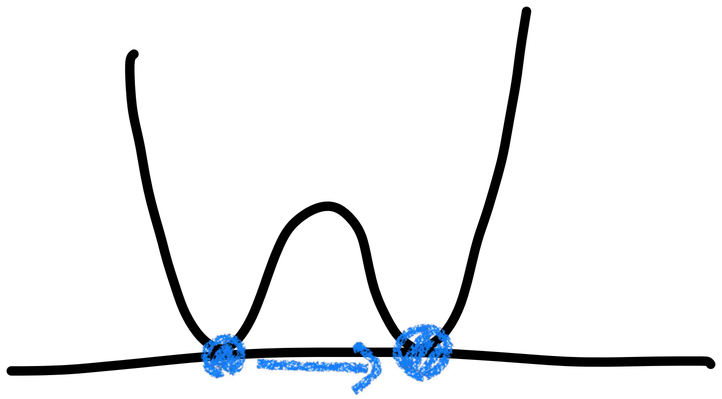
This classical solution is the instanton.

Everything looks nice.

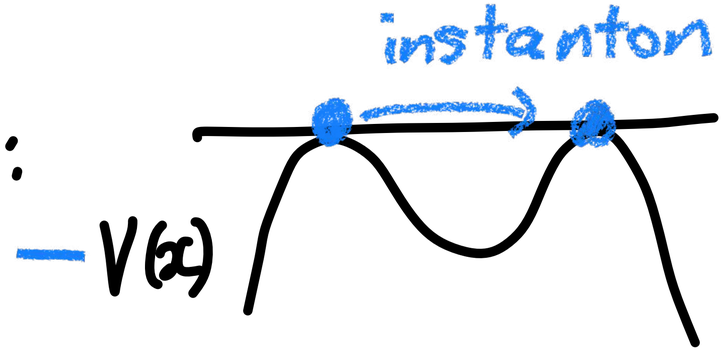
What's the problem?

Q.) Can we understand the tunneling in real-time path integral ?

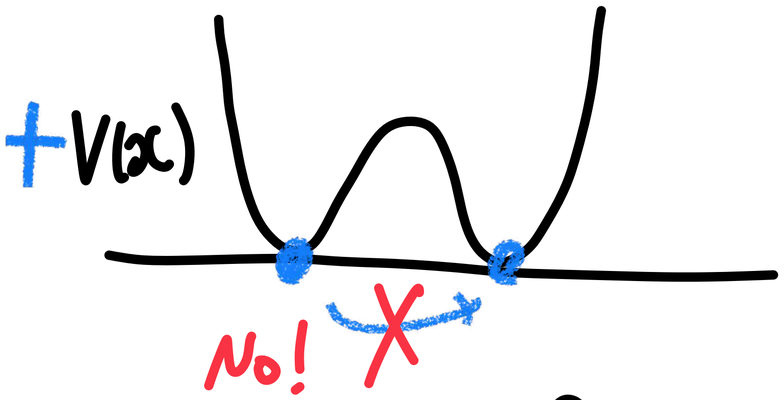
⇝ This is quite difficult.



Such a Real classical solution does not exist.

Imaginary-time : 

⇝ Quantum tunneling is a semiclassical phenomenon.

Real-time : 

⇝ No semiclassical way for tunneling.

Isn't this puzzling?

Lefschetz-thimble path integral

Oscillatory integrals $\Rightarrow \sum_{\sigma}$ (non-oscillatory integrals)

Around 2013-, Lefschetz-thimble method starts getting attention for the sign problem. (Christoforetti, et al '13; Fujii, et al '13-, ... (Witten '10))

$$\int_{\mathbb{R}^{[0,T]}} \mathcal{D}x \; e^{iS[x]} = \sum_{\sigma:\ \text{complex classical sol.}} n_\sigma \int_{J_\sigma} \mathcal{D}z \; e^{iS[z]} .$$

J_σ: Lefschetz thimble

$\approx$ steepest-descent path.

Assume we are interested in the integral

$$Z = \int_{\mathcal{M}} d^n x \quad \exp\left(\frac{1}{\hbar} I(x)\right)$$

($\mathcal{M} = \mathbb{R}^{[0,T]}$, $I(x) = i\,S[x]$ in the real-time path integral)

Complexification $\quad \mathcal{M} \to \mathcal{M}_{\mathbb{C}} = \mathcal{M} \otimes \mathbb{C}$, $\quad x \to z = x + iy$

Convergent Region $\quad C_{-T} = \left\{ z \in \mathcal{M}_{\mathbb{C}} \;\middle|\; \mathrm{Re}(I(z)) < -T \right\}$

Then, Lefschetz thimbles $\quad J_\sigma = \left\{ z(0) \in \mathcal{M}_{\mathbb{C}} \;\middle|\; \frac{dz}{dt} = -\overline{\left(\frac{\partial I}{\partial z}\right)},\ z(-\infty) = z_\sigma \right\}$

(classical sol. $\frac{\partial I}{\partial z} = 0$)

form the basis of $H_n(\mathcal{M}_{\mathbb{C}}, C_{-T})$ for $T \gg 1$.

$$\rightsquigarrow Z = \sum_\sigma n_\sigma \int_{J_\sigma} d^n z \quad \exp\left(\frac{1}{\hbar} I(z)\right).$$

- Integration on each Lefschetz thimble behaves as

$$Z_\sigma := \int_{J_\sigma} d^n z\, e^{\frac{1}{\hbar} I(z)} = e^{\frac{1}{\hbar} I(z_\sigma)} A_0 \hbar^{\textcircled{\scriptsize ?}} \left(1 + a_1 \hbar + \cdots\right)$$

$\rightsquigarrow$ Asymptotic expansion in $\hbar \ll 1$.

Let's apply this method to quantum tunneling!

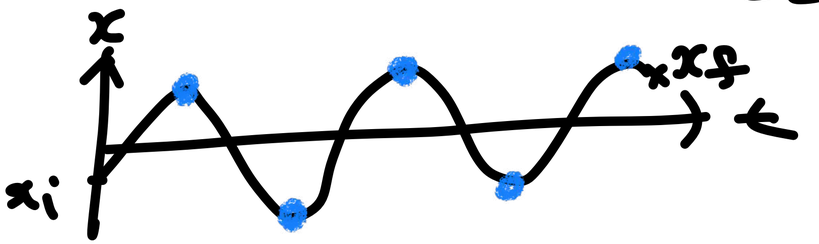
(as it was a semiclassical phenomenon in imaginary time)

(* Use of complex solutions is not a new idea.
But, Lefschetz thimbles may provide a systematic treatment.)

Simple example: Harmonic oscillator

$$I[z] = i\,S[z] = i\int_0^T dt\left\{\frac{1}{2}\left(\frac{dz}{dt}\right)^2 - \frac{1}{2}z^2\right\}.$$

$z_{cl} = x_{cl}$



$$\langle x_f | e^{-i\hat{H}T/\hbar} | x_i \rangle = \sqrt{\frac{1}{2\pi i\hbar\,|\sin(T)|}}\; e^{\frac{I(z_{cl})}{\hbar}} \times e^{-i\frac{\pi}{2}\nu}$$

← Maslov index $= \left\lfloor \frac{T}{\pi} \right\rfloor$

$\int \mathcal{D}x \Rightarrow \int_J \mathcal{D}z$ produces the correct phase factor.

Path toward quantum tunneling

Double-well : $I[z] = i\,S[z] = i\int dt \left(\frac{1}{2}\left(\frac{dz}{dt}\right)^2 - \frac{1}{2}(z^2-1)^2\right)$.

Let's look at behaviors of complex classical solutions.

Energy conservation :

$$\left(\frac{dz}{dt}\right)^2 + (z^2-1)^2 = p^2$$

(p^2: (complex) energy)

$$\Longrightarrow \quad z(t) = \sqrt{\frac{p^2-1}{2p}}\ \mathrm{sd}\left(\sqrt{2p}\,t + c,\ \sqrt{\frac{1+p}{2p}}\right)$$

($k = \sqrt{\frac{1+p}{2p}}$: elliptic modulus)

(sd : Jacobi elliptic func.)

Elliptic function enjoys double periodicity

$\rightsquigarrow$ Set of "classical" paths $x_i \to x_f$ in time T

$$= \left\{ (n,m) \in \mathbb{Z}^2 \quad \text{s.t.} \right.$$

$$\left. n\,\omega_1(k) + m\,\omega_3(k) = \frac{T}{2} + (\text{func. of } x_i, x_f, k) \right\}.$$

with

$$\omega_1(k) = \sqrt{\frac{2k^2-1}{2}}\, K(k) \quad , \quad \omega_3(k) = i\sqrt{\frac{2k^2-1}{2}}\, K(\sqrt{1-k^2}).$$

← complete elliptic integral.

Which solution is responsible for tunneling?

My first naive guess :

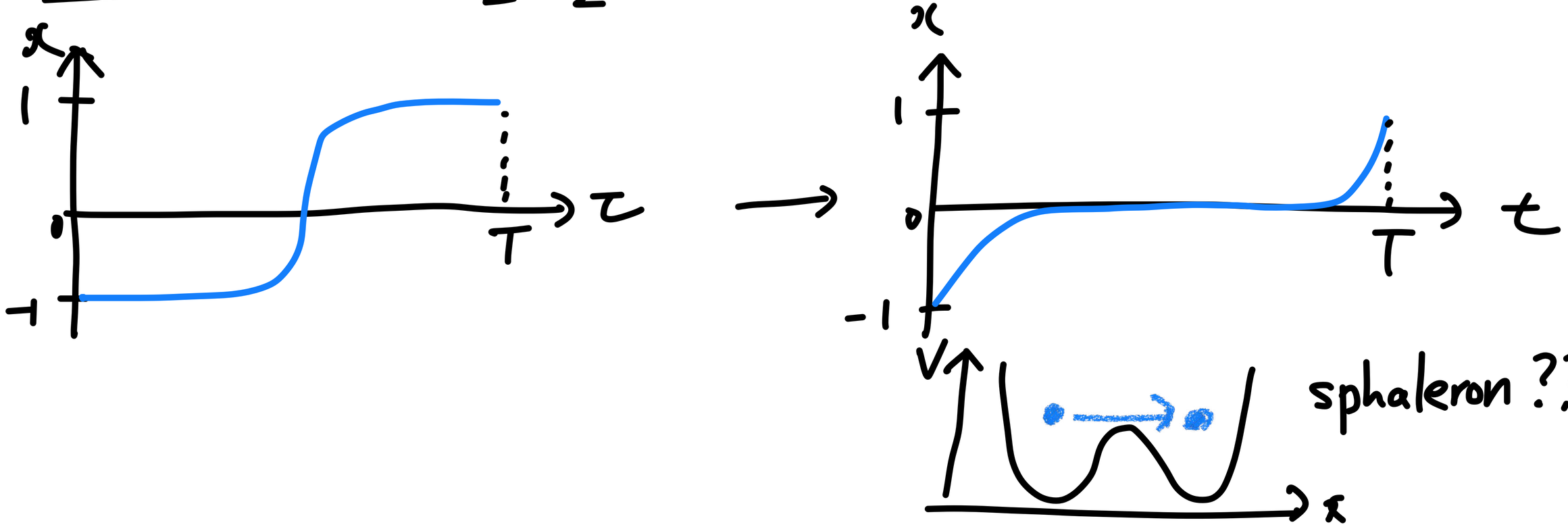
Imaginary-time instanton ⟶ real-time tunneling ?

No !

$n=m=0$

$E=\frac{P^2(k)}{2}\simeq 0$

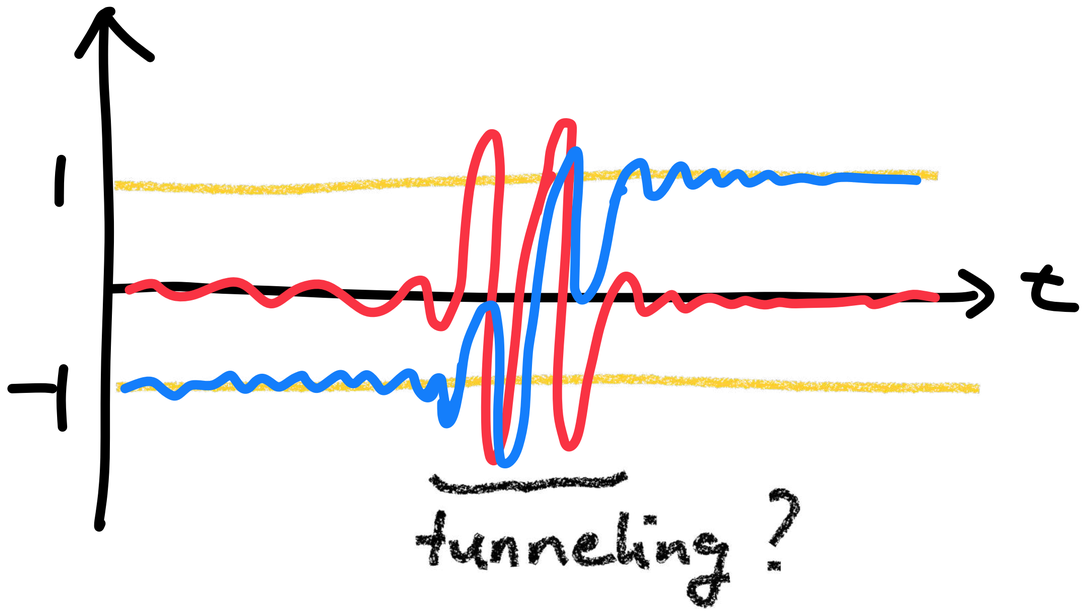
$E=\frac{P^2(k)}{2}\simeq \frac{1}{2}$



sphaleron ??

To find "tunneling-like" sol., $\frac{n}{T}, \frac{m}{T} \sim \mathcal{O}(1)$.

↳ many complex oscillations

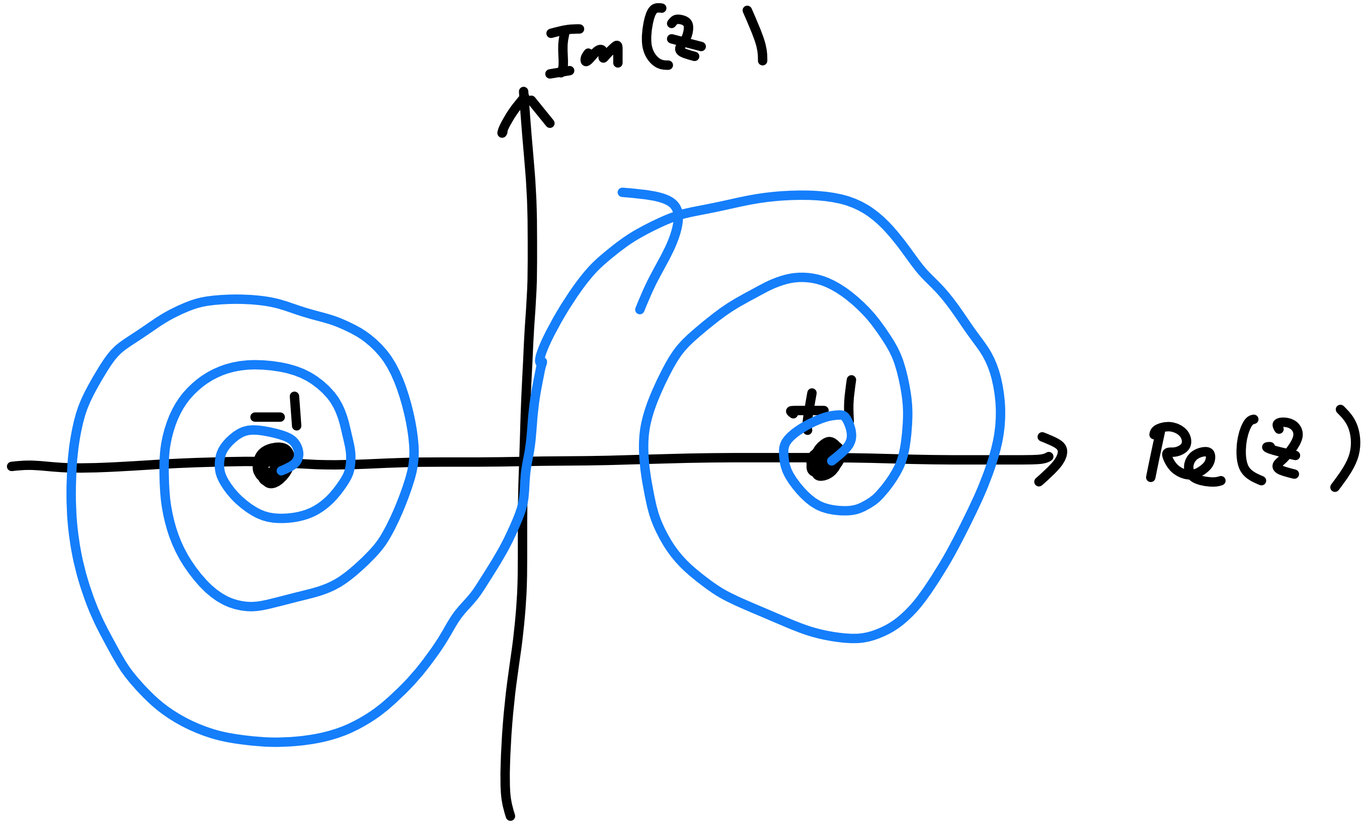


$E \approx 0$.

(cf. Tanizaki, Koike, '14, Cherman, Ünsal, '14)

$$I(z) = i\,S(z) \simeq -\mathcal{O}(1) + i(\text{small imaginary part}).$$

In a complex plane z, it looks like

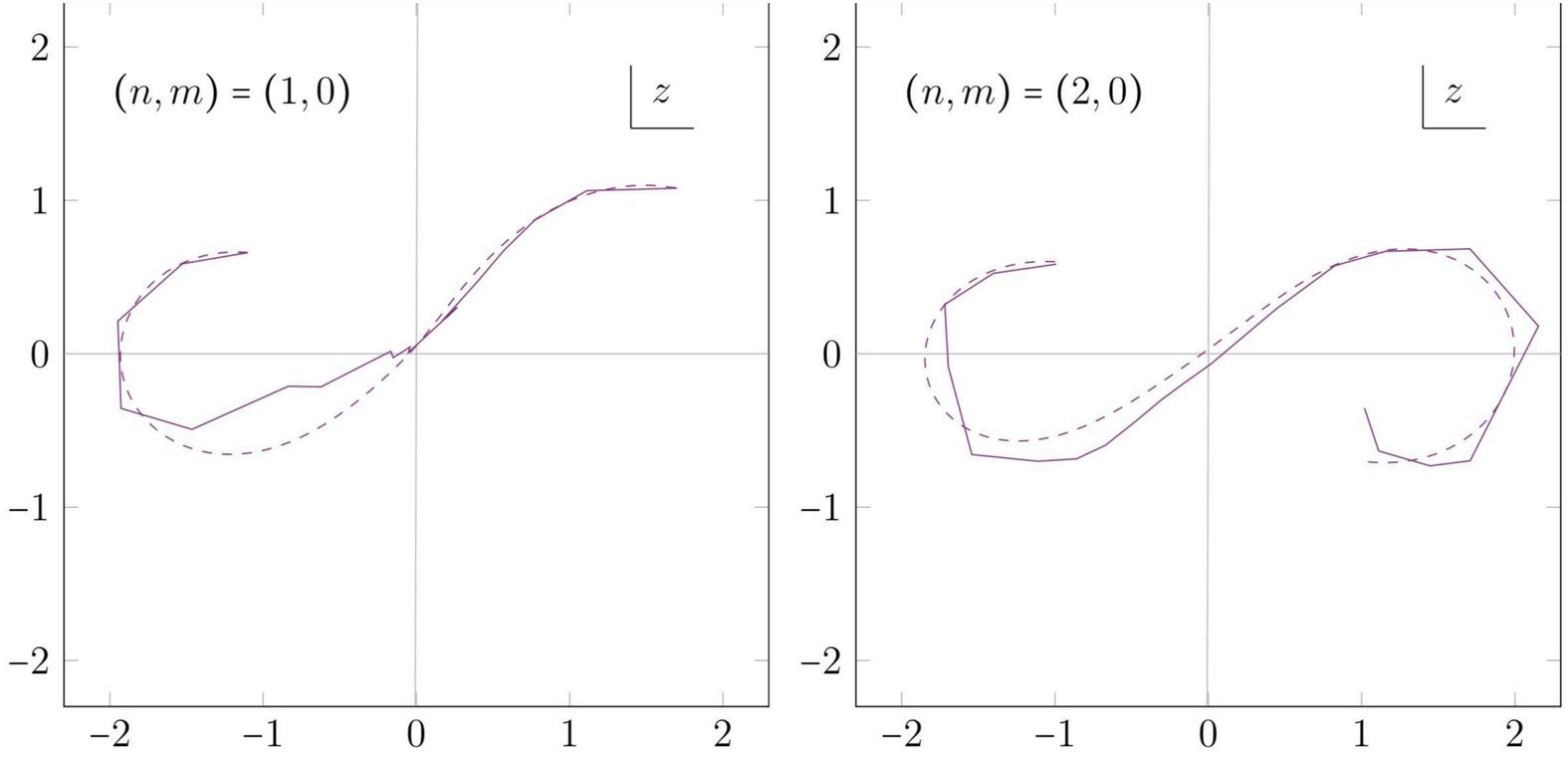


This may be a correct semiclassical view of tunneling.

Recently, Nishimura, Sakai, Yosprakov studied this real-time QM by numerical generalized thimble methods.

They found that such complex trajectories actually appears!!

(Use of gaussian wave packets for initial & final states is important.)



Taken from arXiv:2307.11199

Summary & Future directions

- Lefshetz-thimble path integral may be able to provide a new semi-classical description of the real-time quantum tunneling.
  - Complex classical trajectory seems to play essential roles.
    ↑ This is confirmed in a recent numerical study!

- In this study, we used Dirichlet b.c. as initial and final states.
  ⇒ Preparation of better wave functions may enable us to get easier controll of semiclassics.